

CLAIMS

1. A method for metabolomically facilitating the diagnosis of a disease state of a subject, comprising:
- 5 obtaining a small molecule profile from a subject suspected of having and/or having a disease state; and
- comparing the small molecule profile from the subject to a standard small molecule profile, thereby diagnosing the disease state.
- 10 2. A method for metabolomically predicting whether a subject is predisposed to having a disease state, comprising:
- obtaining a small molecule profile from the subject; and
- comparing the small molecule profile from the subject to a standard small molecule profile, thereby predicting whether a subject is predisposed to having a disease
- 15 state.
3. A method for metabolomically predicting a subject's response to a therapeutic agent, comprising:
- obtaining a small molecule profile from the subject;
- 20 comparing the small molecule profile of the subject to a known standard established for the therapeutic agent as an indication of whether the subject would benefit from treatment with the therapeutic agent, thereby predicting a subject's response to said therapeutic agent.
- 25 4. A method for metabolomically monitoring the effectiveness of a therapeutic agent in clinical trials, comprising:
- obtaining a small molecule profile from a subject in a clinical trial being treated with a therapeutic agent; and
- monitoring changes in the small molecule profile of the subject as an
- 30 indication of the effectiveness of the therapeutic agent in the subject, thereby monitoring the effectiveness of said therapeutic agent.
5. The method of any one of claims 1-4, wherein said subject is a human.
- 35 6. The method of any one of claims 1-4, wherein said subject is suffering or suspected of suffering from a disease state.

TECHNOLOGICAL

5

9.

10.

11.

12.

13.

14.

15.

16.

35

of claim 8, where

of claim 8, where

logical, metabolic

of claim 8, where

's liver, heart, m

e.

10

15

20

25

30

35

~~in claim 20.~~

27. A method for identifying small molecules affected by an agent comprising:

5 obtaining a small molecule profile of said cellular compartment
treated with an agent, and
comparing said small molecule profile to a standard small
molecule profile;
thereby, identifying the compounds affected by said agent in said
cellular compartment.

10

28. The method of claim 27, wherein said agent is a toxin.

29. The method of claim 27, wherein said agent is a therapeutic agent.

15 ~~30. The method of claim 29, wherein said therapeutic agent is a therapeutic agent used for the treatment of a metabolic, immunological, neurological, oncological, viral, or other disorder.~~

20 ~~31. The method of claim 27, wherein said cellular compartment is obtained from a patient.~~

~~32. The method of claim 31, wherein said patient is suffering from a metabolic, immunological, neurological, oncological, viral, or other disorder.~~

25 ~~33. The method of claim 27, wherein said cellular compartment is a cells.~~

~~34. The method of claim 27, wherein said cellular compartment is mitochondria.~~

30 ~~35. The method of claim 27, wherein said cellular compartment is a nucleus.~~

36. The method of claim 27, wherein said small molecule profiles are obtained using one or more of the following: HPLC, TLC, electrochemical analysis, mass spectroscopy, refractive index spectroscopy (RI), Ultra-Violet spectroscopy (UV),
35 fluorescent analysis, radiochemical analysis, Near-InfraRed spectroscopy (Near-IR), Nuclear Magnetic Resonance spectroscopy (NMR), and Light Scattering analysis (LS).

098560
04130
Sub A2

37. A method for identifying small molecules regulated, modulated, or associated with a gene, comprising:

obtaining a small molecule profile of a cellular compartment from a genetically modified source; and

5 comparing the small molecule profile to a standard small molecule profile, thus identifying the small molecules regulated, modulated or associated with the gene.

Sub A3
10 38. The method of claim 37, wherein said cellular compartment is a cells.

39. The method of claim 37, wherein said cellular compartment is a mitochondria.

40. The method of claim 37, wherein said cellular compartments is a nucleus.

15 41. The method of claim 37, wherein said genetic modification is an expression vector.

42. The method of claim 41, wherein said expression vector is a portion of
20 the human genome.

43. The method of claim 42, wherein said expression vector is associated with a particular disease state.

25 44. A method for identifying potential cell drug targets, comprising:
contacting a labeled disease relevant small molecule with cellular components; and
identifying interactions between said cell components and the labeled disease-relevant small molecule, thus identifying potential cell drug targets.

30 45. The method of claim 44, wherein said cellular components are a nucleic acid array.

46. The method of claim 44, wherein said cellular components are a protein
35 array.

47. The cellular components identified by the method of claim 44.

09835119.044304
TOCTHO-6TTS660

Sub A4

48. A library of small molecules of a cellular compartment of a cell comprising a searchable array of samples of small molecules from a cellular compartment.

5

49. The library of claim 48, wherein said small molecules are isolated.

50. The library of claim 48, wherein said cell is an animal cell.

10 51. The library of claim 48, wherein said cellular compartment is a mitochondria.

52. The library of claim 48, wherein said cellular compartment is a nucleus.

15 53. The library of claim 48, wherein said cellular compartment is a chloroplast.

54. A method for determining whether small molecule profiles are from the same individual, comprising:

20

obtaining one or more samples from an individual;
determining the small molecule profiles of said samples;
obtaining a tissue sample from an unknown source;
determining the small molecule profile of the unknown source; and
comparing the small molecule profiles, thus determining whether the

25 small molecule profiles are from the same individual.

Sub A5

55. A pharmaceutical composition comprising a small molecule identified by the method of claim 1.